

So called Heusler compounds of transition metals are vast class of materials with wide gamut of physicochemical properties, which can be broadly applied in spintronics and renewable sources of energy. They were intensively studied for many years and displayed giant magnetoresistance, outstanding photovoltaic properties, shape memory, magnetocaloric and thermoelectric effects, and strong electron correlations. They can be magnetic semiconductors, semimetals, or half-metals, magnetically ordered materials, or superconductors. These multifunctional properties can be easily tuned with small modifications of their composition or various external parameters.

Discovery of three-dimensional topological systems in the first decade of this century triggered extremely dynamic development of a new branch of physics dealing with topological materials. Nowadays, numerous insulators and semimetals possessing non-trivial metallic states protected against chaotic perturbations by topological constraints, are intensively studied by advanced experimental and theoretical methods of physics, chemistry and material science.

During last ten years, intense studies by ours and other groups, have shown that many of compounds belonging to a subclass of rare-earth based half-Heusler phases are topological insulators or semimetals, and simultaneously possess many of aforementioned multifunctional properties. Such a meeting of topological non-triviality with multifunctional properties may result in multifunctional topological material, like topological superconductor, anomalous Hall effect system, dynamical axion, or topological heavy-fermion system. We would like to modify half-Heusler phases by chemical substitution (preparing solid solutions, also with magnetic and non-magnetic atoms substituted with each other) and/or obtaining them in form of thin films. Such modifications will allow us to tune, enhance and even generate novel multifunctional topological properties.

In order to predict the impact of structural modifications on electronic state we will use results of first-principles electronic structure calculations, both our own and previously reported. Combining our complementary vast experience in single-crystal growth (from fluxes) and thin-film preparation (by co-sputtering, evaporation or pulse laser deposition) of half-Heusler phases, measurements of electronic (magnetoresistance, Hall effect, quantum oscillations) and magnetic properties, profound characterization of superconducting state (resistivity, magnetic susceptibility, specific heat) at very low temperatures will bring us thorough understanding and effective fine-tuning of multifunctional topological properties resulting from correlations of the structure, chemical composition and bulk magnetism with electronic structure and spin-orbit coupling. Devices based on the optimized multifunctional topological thin films will be fabricated and characterized.

Special effort will be devoted to characterization of topological superconductivity observed in half-Heusler compounds at very low temperatures and even coexisting with magnetically ordered state. In non-magnetic YPtBi a new type of pairing-mixed state was found, namely the mixture of s-wave spin-singlet and d-wave spin-quintet channels, induced by spin-orbit coupling even in the absence of inversion symmetry, when electrons carry effective "spin-3/2". Topological superconductivity is extremely interesting state of quantum matter, being associated with fascinating quasiparticle excitations: Majorana fermions.

We will try to observe and prove the bulk band structure of half-Heusler compounds and reveal the effect of strength of spin-orbit coupling on the bulk electronic band structure. Instead of surface-sensitive methods, such as angle-resolved photoemission spectroscopy and scanning tunneling spectroscopy, we will use the bulk-sensitive nuclear magnetic resonance spectroscopy to reveal ^{209}Bi isotropic shifts scale-relative to the magnitude of spin-orbit coupling and average atomic numbers.

The complementary expertise of our groups creates a powerful and versatile joint team which has all required skills and facilities to cope with the challenges of the proposed technology. This project will have broad ramifications for both fundamental research and potential applications and is expected to stimulate future joint research.

The expected outcome of the project will be initiation of new original research pathways in the blooming physics of topological matter. Exploration and deep understanding the role magnetism plays in magnetic topological insulators and semimetals, in particular its interplay with superconductivity, will not only substantially expand our knowledge, but potentially will bring novel applications of such materials in design and fabrication of memory units, sensors, magnetic switches and other spintronic devices, and possibly also innovative devices for quantum computing.